L Number	Hits	Search Text	DB	Time stamp
1	697	544/71, 544/101, 514/230.2	USPAT	2004/10/27 13:58
2	80834	microbial or microb$	USPAT	2004/10/27 13:58
3	70	(544/71, 544/101, 514/230.2) and (microbial or microb$)	USPAT	2004/10/27 13:58

Day : Wednesday
Date: 10/27/2004
Time: 13:59:14

PALM INTRANET

Inventor Information for 10/677551

Inventor Name	City	State/Country
BARBACHYN, MICHAEL ROBERT	ANN ARBOR	MICHIGAN
RUBLE, J. CRAIG	GREENWOOD	INDIANA
ROMERO, ARTHUR GLENN	CHESTERFIELD	MISSOURI
THOMASCO, LISA MARIE	GROTON	CONNECTICUT
HURD, ALEXANDER ROSS	ANN ARBOR	MICHIGAN
PALMER, JOHN RAYMOND	FISHERS	INDIANA
TOOGOOD, PETER LAURENCE	ANN ARBOR	MICHIGAN
MCNAMARA, DENNIS JOSEPH	ANN ARBOR	MICHIGAN
SHERRY, DEBRA ANN	CHELSEA	MICHIGAN
DOBROWOLSKI, PAUL JOSEPH	SALINE	MICHIGAN

Appln Info | Contents | Petition Info | Atty/Agent Info | Continuity Data | Foreign Data

Search Another: Application# Search **or Patent#** Search

PCT / / Search **or PG PUBS #** Search

Attorney Docket # Search

Bar Code # Search

To go back use Back button on your browser toolbar.

Back to PALM | ASSIGNMENT | OASIS | Home page

h e eb cg b e e f e

(2)

	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:52:16 ON 27 OCT 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 26 OCT 2004 HIGHEST RN 769912-90-5
DICTIONARY FILE UPDATES: 26 OCT 2004 HIGHEST RN 769912-90-5

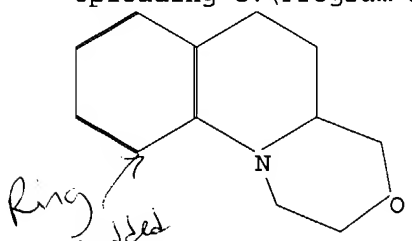
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

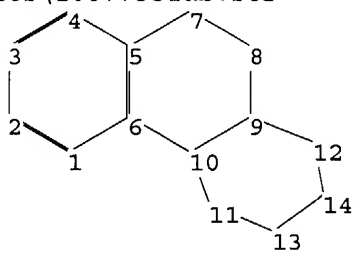
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10677551ab.str



Ring embedded



ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 9-12 10-11 11-13 12-14 13-14
exact/norm bonds :
5-7 6-10 7-8 8-9 9-10 9-12 10-11 11-13 12-14 13-14
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom

L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 11:52:32 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 882 TO ITERATE

100.0% PROCESSED 882 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 15859 TO 19421
PROJECTED ANSWERS: 7 TO 298

L2 7 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 11:52:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 16937 TO ITERATE

100.0% PROCESSED 16937 ITERATIONS 158 ANSWERS
SEARCH TIME: 00.00.01

L3 158 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 155.42 155.63

FILE 'CAPLUS' ENTERED AT 11:52:56 ON 27 OCT 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 27 Oct 2004 VOL 141 ISS 18
FILE LAST UPDATED: 26 Oct 2004 (20041026/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

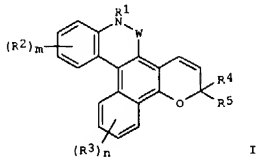
=> s l3
L4 11 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:778888 CAPLUS
DOCUMENT NUMBER: 141:278615
TITLE: Photochromic chromenes showing rapid decoloration, and optical materials containing them
INVENTOR(S): Izumi, Shinobu; Yamamoto, Hiromasa
PATENT ASSIGNEE(S): Tokuyama Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004262837	A2	20040924	JP 2003-54827	20030228
PRIORITY APPLN. INFO.:			JP 2003-54827	20030228

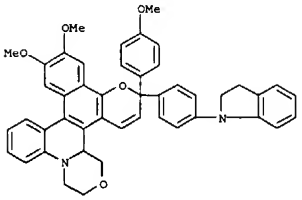
GI



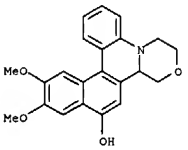
I

AB Photochromic optical materials (e.g., lenses) contain chromenes I [W = (un)substituted (cyclo)alkylene, (un)substituted arylene; R1 = H, alkyl, aralkyl; R1 may form ring with W; R2, R3 = OH, alkyl, alkoxy, aralkyl, aralkoxy, amino, cyano, NO2, etc.; R4, R5 = alkyl, (un)substituted aryl, aromatic heterocyclyl; R4R5 may form ring; m, n = 0-4]. Thus, tetraethylene glycol dimethacrylate, 2,2-bis[4-(methacryloyloxyethoxy)phenyl]propane, polyethylene glycol monoallyl ether, trimethylolpropane trimethacrylate, and glycidyl methacrylate were polymerized in the presence of I [R1W = (CH2)4CH, R4 = C6H4NMe2-p, R5 = Ph, m = n = 0] in a mold to give a polymer material showing λmax 592 nm, coloration d. [ε(120) - ε(0)] 0.88, decoloration rate (t1/2) 22 s, and inital yellowness index 4.

IT **758691-63-3P**
RL: IMF (Industrial manufacture); MOA (Modifier or additive use); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(manuf. of photochromic chromenes for lenses)
RN 758691-63-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



IT **758691-72-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(manufacture of photochromic chromenes for lenses)
RN 758691-72-4 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

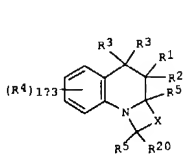


own work

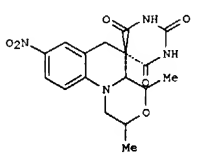
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:308443 CAPLUS
DOCUMENT NUMBER: 140:339202
TITLE: Preparation of tricyclic tetrahydroquinoline antibacterial agents
INVENTOR(S): Barbachyn, Michel Robert; Dobrowolski, Paul Joseph; Hurd, Alexander Ross; McNamara, Dennis Joseph; Palmer, John Raymond; Romero, Arthur Glenn; Ruble, James Craig; Sherry, Debra Ann; Thomasco, Lisa Marie; Toogood, Peter Laurence
PATENT ASSIGNEE(S): Pharmacia & Upjohn Company, USA
SOURCE: PCT Int. Appl., 128 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031195	A1	20040415	WO 2003-IB4389	20031003
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004162279	A1	20040819	US 2003-677551	20031002
PRIORITY APPLN. INFO.:			US 2002-416685P P	20021007
			US 2002-427189P P	20021118
			US 2003-457622P P	20030326

OTHER SOURCE(S): MARPAT 140:339202
GI



I



II

AB The invention includes tricyclic tetrahydroquinolines (shown as I;

L4 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(Preparation); USES (Uses)
(manuf. of photochromic chromenes for lenses)
RN 758691-63-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

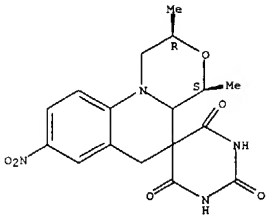
IT **758691-72-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(manufacture of photochromic chromenes for lenses)
RN 758691-72-4 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
variables defined below; many of the examples are spiro compds., e.g. cis- and trans-II), and pharmaceutical compns. thereof, that exhibit useful antibacterial activity against a wide range of human and veterinary pathogens. For I: R1 is R12, C(O)R6, or CN; R2 = R12, C(O)R7, CN, CH2R7, NR17R7, CH2COR7, CH2CH2COR7; R3 = H, R2, O, C1-7 alkyl, C3-8 cycloalkyl, aryl, heteroaryl, or halo; each R4 = H, halo, OR12, OC(O)NR9R10, SR12, S(O)mR13, NR9R10, NR9S(O)mR13, NR9C(O)OR13, Ph, heteroaryl, cyano, nitro, CONR9R10, CO2R12, C(O)R13, C(:NOR12)R13, S(O)mNR9R10, NR9C(O)R12, C1-7 alkyl, C3-8 cycloalkyl, N3, hetl, or C(O)O-C1-4alkyl-R12; each R5 = H, C1-7alkyl, C3-8cycloalkyl, aryl or heteroaryl;. X = -[C(R15)2]n-, -[C(R15)2]m-O-[C(R15)2]k-, -[C(R15)2]m-S(O)m-[C(R15)2]k-, or -[C(R15)2]m-NR16-[C(R15)2]k-; R20 is H, C1-7alkyl, C3-8cycloalkyl, aryl, or heteroaryl; Hetl is a C- or N-linked 5-8 membered mono- or bicyclic ring, each mono- or bicyclic ring being fully satd. or partially unsatd., and having 1-4 heteroatoms O, S, and N; hetl being (un)substituted by 1-2 substituents = C1-C4alkyl, amino, C1-C4alkylamino, C1-C4alkyloxy, halogen, CN, O, or S; addnl. details including provisos are given in the claims. A method of prepn. is claimed and .apprx.60 example prepns. are included. For example, cis- and trans-II were prepd. in 3 steps starting with condensation of 2-fluoro-5-nitrobenzaldehyde with 2,6-dimethylmorpholine to give cis- and trans-2-(2,6-dimethylmorpholin-4-yl)-5-nitrobenzaldehyde, each of which was condensed with barbituric acid to give cis- and trans-5-[2-(2,6-dimethylmorpholin-4-yl)-5-nitrobenzylidene]pyrimidine-2,4,6(1H,3H,5H)-trione, resp., each of which was cyclized in refluxing MeOH. Inhibition of E. coli DNA gyrase by 12 examples of I are reported.

IT **679839-05-5P**
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(drug candidate, chromatog. resolution; preparation of tricyclic tetrahydroquinoline antibacterial agents)
RN 679839-05-5 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-, (2R,4S)-rel- (9CI) (CA INDEX NAME)

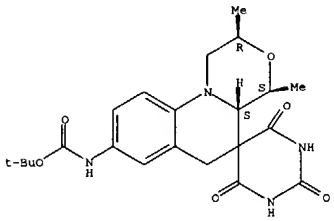
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **679839-36-2P 679839-41-9P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of tricyclic tetrahydroquinoline antibacterial agents)
RN 679839-36-2 CAPLUS
CN Carbamic acid, [(2R,4S,4aS)-1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-8-yl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

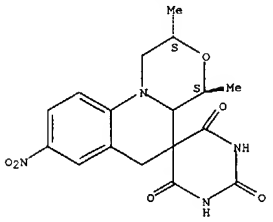
Relative stereochemistry.



RN 679839-41-9 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-acetyl-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

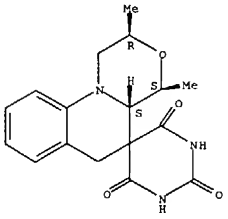
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
679840-95-0P 681006-33-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; prepn. of tricyclic tetrahydroquinoline antibacterial agents)
RN 679839-06-6 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-, (2R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



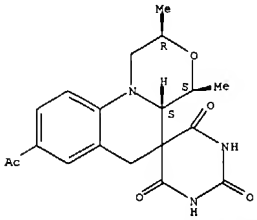
RN 679839-11-3 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



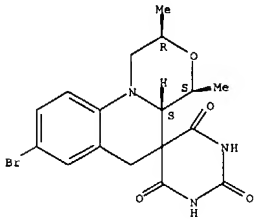
RN 679839-13-5 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Relative stereochemistry.



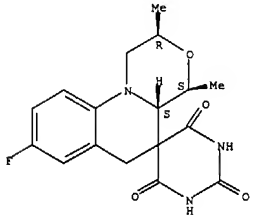
IT **679839-06-6P 679839-11-3P 679839-13-5P**
679839-16-8P 679839-19-1P 679839-22-6P
679839-24-8P 679839-26-0P 679839-27-1P
679839-31-7P 679839-33-9P 679839-34-0P
679839-35-1P 679839-37-3P 679839-38-4P
679839-44-2P 679839-45-3P 679839-48-6P
679839-50-0P 679839-52-2P 679839-55-5P
679839-56-6P 679839-57-7P 679839-58-8P
679839-63-5P 679839-64-6P 679839-65-7P
679839-68-0P 679839-71-5P 679839-73-7P
679839-74-8P 679839-76-0P 679839-78-2P
679839-80-6P 679839-82-8P 679839-83-9P
679839-84-0P 679839-87-3P 679839-92-0P
679839-99-7P 679840-05-2P 679840-13-2P
679840-15-4P 679840-19-8P 679840-23-4P
679840-25-6P 679840-29-0P 679840-31-4P
679840-32-5P 679840-33-6P 679840-34-7P
679840-35-8P 679840-36-9P 679840-37-0P
679840-38-1P 679840-39-2P 679840-40-5P
679840-41-6P 679840-42-7P 679840-43-8P
679840-44-9P 679840-45-0P 679840-46-1P
679840-47-2P 679840-48-3P 679840-49-4P
679840-50-7P 679840-51-8P 679840-52-9P
679840-53-0P 679840-54-1P 679840-55-2P
679840-56-3P 679840-57-4P 679840-58-5P
679840-59-6P 679840-60-9P 679840-61-0P
679840-62-1P 679840-63-2P 679840-64-3P
679840-65-4P 679840-66-5P 679840-67-6P
679840-68-7P 679840-69-8P 679840-70-1P
679840-71-2P 679840-72-3P 679840-74-5P
679840-75-6P 679840-76-7P 679840-77-8P
679840-78-9P 679840-79-0P 679840-80-3P
679840-81-4P 679840-82-5P 679840-83-6P
679840-85-8P 679840-86-9P 679840-88-1P
679840-89-2P 679840-90-5P 679840-91-6P
679840-92-7P 679840-93-8P 679840-94-9P

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Relative stereochemistry.



RN 679839-16-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-fluoro-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

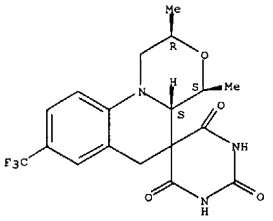
Relative stereochemistry.



RN 679839-19-1 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(trifluoromethyl)-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

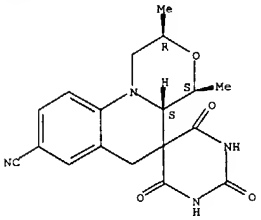
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-22-6 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8-carbonitrile,
1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

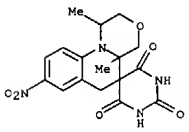
Relative stereochemistry.



RN 679839-24-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8-carboxamide,
1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

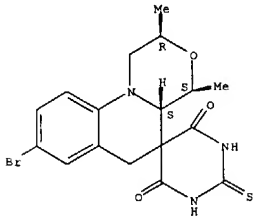
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-33-9 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-4',6'(1'H,3'H)-dione,
8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-2'-thioxo-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

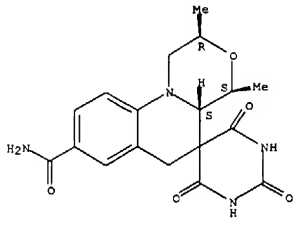
Relative stereochemistry.



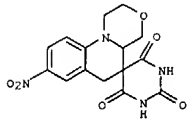
RN 679839-34-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-bromo-1,2,4,4a-tetrahydro-1',2,3',4-tetramethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

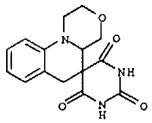
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-26-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-8-nitro- (9CI) (CA INDEX NAME)

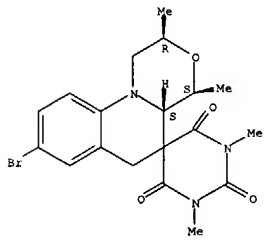


RN 679839-27-1 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro- (9CI) (CA INDEX NAME)



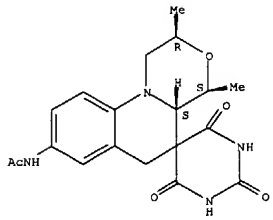
RN 679839-31-7 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-1,4a-dimethyl-8-nitro- (9CI)
(CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-35-1 CAPLUS
CN Acetamide, N-[(2R,4S,4aS)-1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-8-yl]-, rel- (9CI) (CA INDEX NAME)

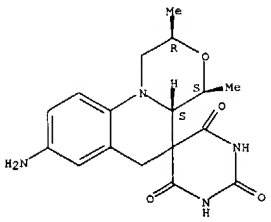
Relative stereochemistry.



RN 679839-37-3 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-amino-1,2,4,4a-tetrahydro-2,4-dimethyl-, monohydrochloride, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

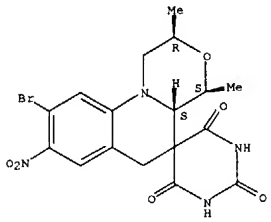
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



● HCl

RN 679839-38-4 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 9-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

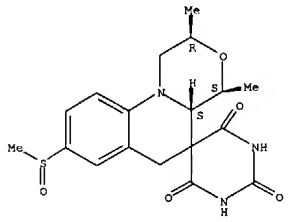
Relative stereochemistry.



RN 679839-44-2 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-8-[1-(methoxyimino)ethyl]-2,4-dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

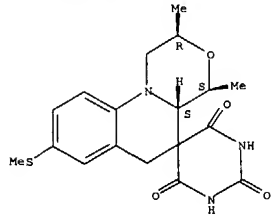
Relative stereochemistry.
Double bond geometry unknown.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-50-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(methylthio)-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

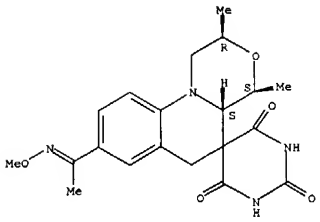
Relative stereochemistry.



RN 679839-52-2 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-nitro-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

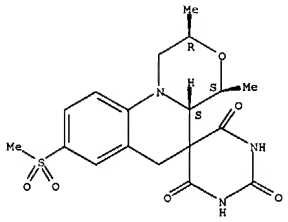
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-45-3 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(methylsulfonyl)-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

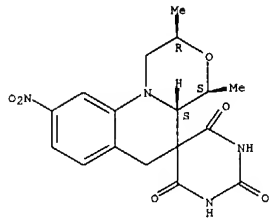
Relative stereochemistry.



RN 679839-48-6 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(methylsulfinyl)-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

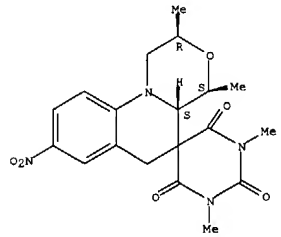
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-55-5 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-1',2,3',4-tetramethyl-8-nitro-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

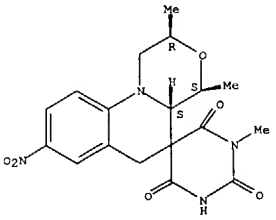
Relative stereochemistry.



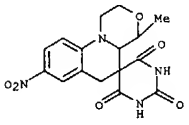
RN 679839-56-6 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-1',2,4-trimethyl-8-nitro-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

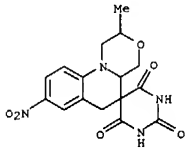
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



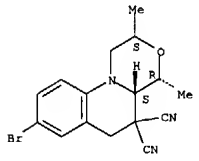
RN 679839-57-7 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-4-methyl-8-nitro- (9CI) (CA INDEX NAME)



RN 679839-58-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2-methyl-8-nitro- (9CI) (CA INDEX NAME)

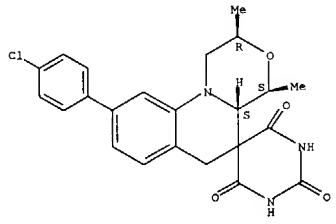


L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-68-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 9-(4-chlorophenyl)-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

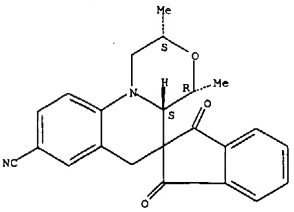


RN 679839-71-5 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-[4-(trifluoromethoxy)phenyl]-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

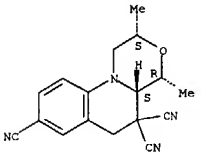
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 679839-63-5 CAPLUS
CN Spiro[2H-indene-2,5'(6'H)-[1,4]oxazino[4,3-a]quinoline]-8'-carbonitrile, 1,1',2',3,4',4'a-hexahydro-2',4'-dimethyl-1,3-dioxo-, (2'R,4'S,4'aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 679839-64-6 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5,8(6H)-tricarbonitrile, 1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aR)-rel- (9CI) (CA INDEX NAME)

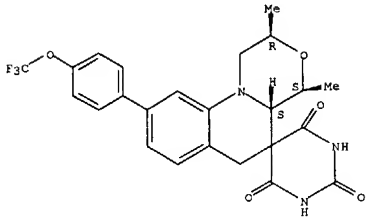
Relative stereochemistry.



RN 679839-65-7 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aR)-rel- (9CI) (CA INDEX NAME)

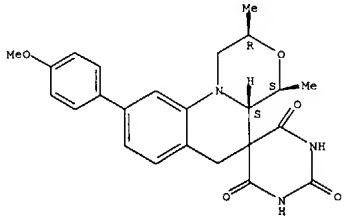
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-73-7 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-9-(4-methoxyphenyl)-2,4-dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

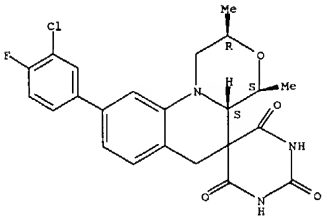
Relative stereochemistry.



RN 679839-74-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 9-(3-chloro-4-fluorophenyl)-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

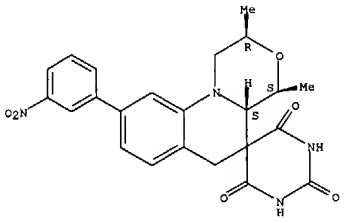
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-76-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-(3-nitrophenyl)-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

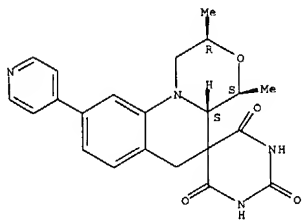
Relative stereochemistry.



RN 679839-78-2 CAPLUS
CN Benzonitrile, 4-[(2R,4S,4aS)-1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-9-yl]-, rel- (9CI) (CA INDEX NAME)

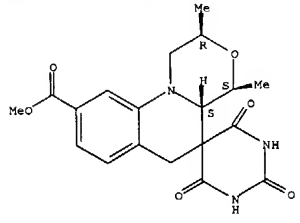
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-83-9 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-9-carboxylic acid, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-, methyl ester, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

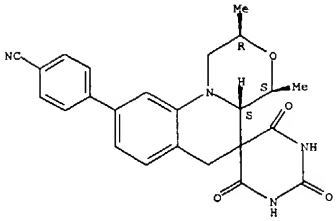
Relative stereochemistry.



RN 679839-84-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8-carboxylic acid, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-, methyl ester, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

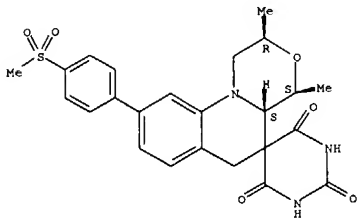
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-80-6 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-[4-(methylsulfonyl)phenyl]-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

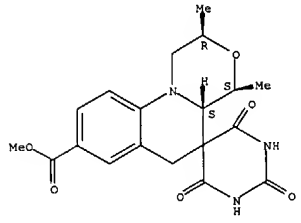
Relative stereochemistry.



RN 679839-82-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-(4-pyridinyl)-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

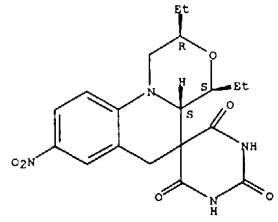
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-87-3 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 2,4-diethyl-1,2,4,4a-tetrahydro-8-nitro-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

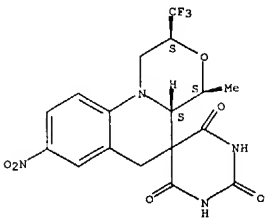
Relative stereochemistry.



RN 679839-92-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-4-methyl-8-nitro-2-(trifluoromethyl)-, (2R,4R,4aR)-rel- (9CI) (CA INDEX NAME)

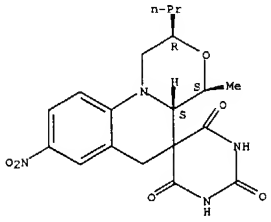
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-99-7 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-4-methyl-8-nitro-2-propyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

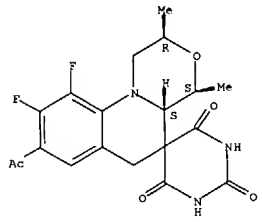
Relative stereochemistry.



RN 679840-05-2 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-, (2S,4S,4aS)- (9CI) (CA INDEX NAME)

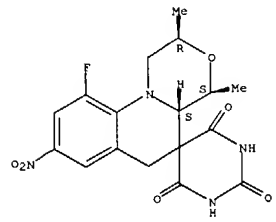
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-19-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 10-fluoro-1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

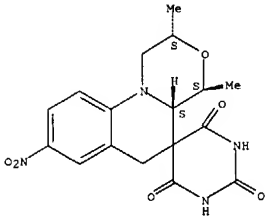
Relative stereochemistry.



RN 679840-23-4 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(5-methyl-1,2,4-oxadiazol-3-yl)-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

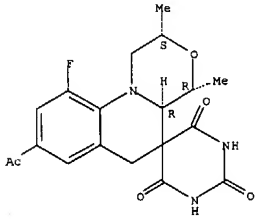
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-13-2 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-acetyl-10-fluoro-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

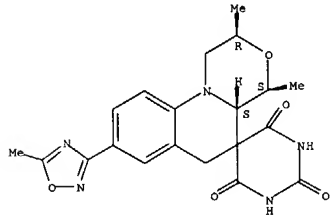
Relative stereochemistry.



RN 679840-15-4 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-acetyl-9,10-difluoro-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

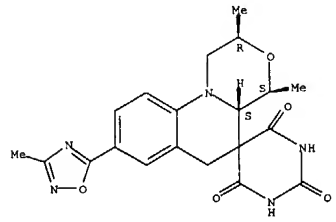
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-25-6 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(3-methyl-1,2,4-oxadiazol-5-yl)-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

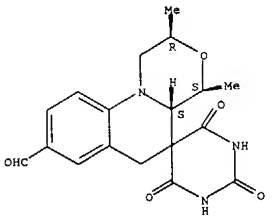
Relative stereochemistry.



RN 679840-29-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8-carboxaldehyde, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

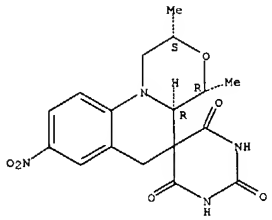
Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



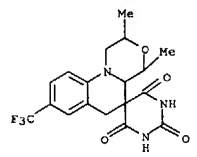
RN 679840-31-4 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-, (2R,4S,4aS)-rel-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

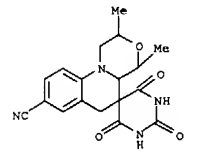


RN 679840-32-5 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

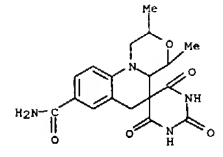
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 679840-36-9 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8-carbonitrile,
1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo- (9CI) (CA INDEX NAME)

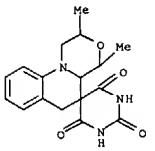


RN 679840-37-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8-carboxamide, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo- (9CI) (CA INDEX NAME)

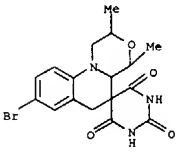


RN 679840-38-1 CAPLUS
CN Acetamide, N-(1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-8-yl)-

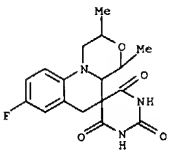
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-33-6 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

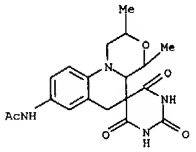


RN 679840-34-7 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-fluoro-1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

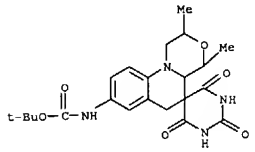


RN 679840-35-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-

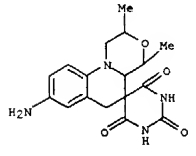
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(9CI) (CA INDEX NAME)



RN 679840-39-2 CAPLUS
CN Carbamic acid, (1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-8-yl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



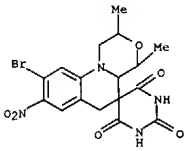
RN 679840-40-5 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-amino-1,2,4,4a-tetrahydro-2,4-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



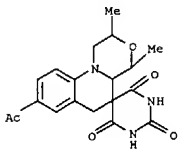
● HCl

RN 679840-41-6 CAPLUS

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 9-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro- (9CI) (CA INDEX NAME)

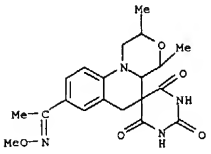


RN 679840-42-7 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-acetyl-1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

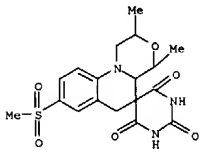


RN 679840-43-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-8-[1-(methoxyimino)ethyl]-2,4-dimethyl- (9CI) (CA INDEX NAME)

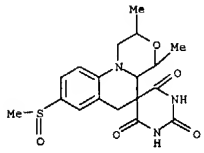
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-44-9 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(methylsulfonyl)- (9CI) (CA INDEX NAME)

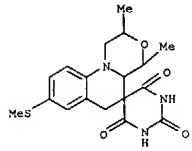


RN 679840-45-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(methylsulfinyl)- (9CI) (CA INDEX NAME)

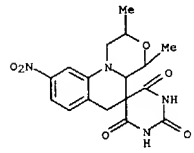


RN 679840-46-1 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(methylthio)-

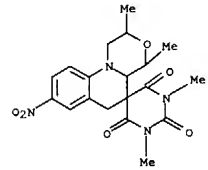
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(9CI) (CA INDEX NAME)



RN 679840-47-2 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-nitro- (9CI) (CA INDEX NAME)

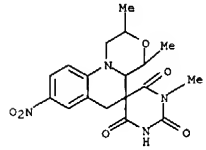


RN 679840-48-3 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-1',2,3',4-tetramethyl-8-nitro- (9CI) (CA INDEX NAME)

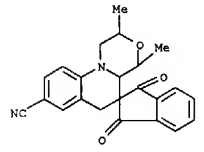


RN 679840-49-4 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-1',2,4-trimethyl-8-nitro- (9CI) (CA INDEX NAME)

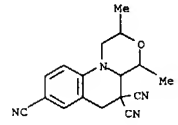
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-50-7 CAPLUS
CN Spiro[2H-indene-2,5'(6'H)-[1,4]oxazino[4,3-a]quinoline]-8'-carbonitrile, 1,1',2',3,4',4'a-hexahydro-2',4'-dimethyl-1,3-dioxo- (9CI) (CA INDEX NAME)

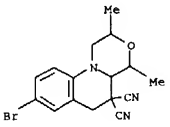


RN 679840-51-8 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5,8(6H)-tricarbonitrile, 1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

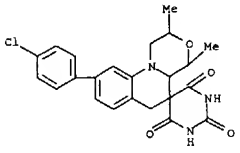


RN 679840-52-9 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

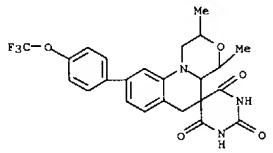
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-53-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 9-(4-chlorophenyl)-1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

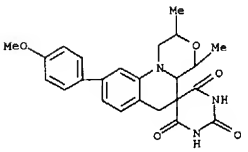


RN 679840-54-1 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-[4-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)

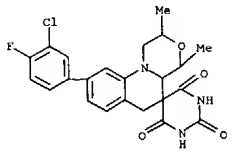


RN 679840-55-2 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-9-(4-methoxyphenyl)-2,4-dimethyl- (9CI) (CA INDEX NAME)

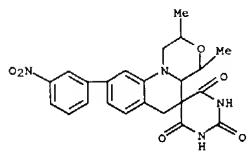
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-56-3 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 9-(3-chloro-4-fluorophenyl)-1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

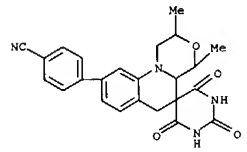


RN 679840-57-4 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

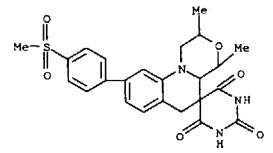


RN 679840-58-5 CAPLUS
CN Benzonitrile, 4-(1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-9-yl)- (9CI) (CA INDEX NAME)

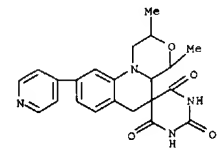
L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-59-6 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

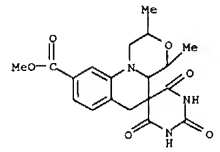


RN 679840-60-9 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-(4-pyridinyl)- (9CI) (CA INDEX NAME)

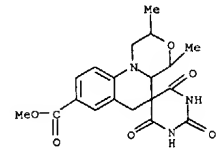


RN 679840-61-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-9-carboxylic acid, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



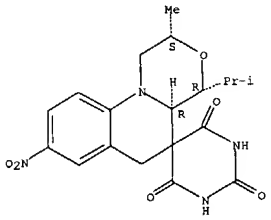
RN 679840-62-1 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8-carboxylic acid, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 679840-63-2 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2-methyl-4-(1-methylethyl)-8-nitro-, (2S,4R,4aR)- (9CI) (CA INDEX NAME)

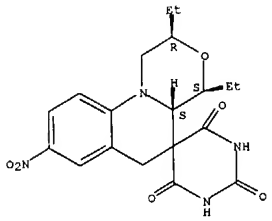
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-64-3 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 2,4-diethyl-1,2,4,4a-tetrahydro-8-nitro-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

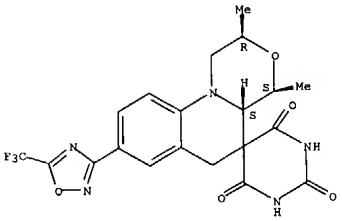
Absolute stereochemistry.



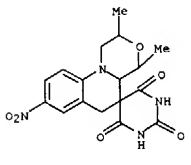
RN 679840-65-4 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-acetyl-9,10-difluoro-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



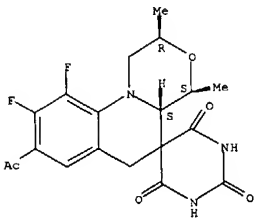
RN 679840-68-7 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro- (9CI) (CA INDEX NAME)



RN 679840-69-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-4-methyl-2-(1-methylethyl)-8-nitro-, (2S,4R,4aR)- (9CI) (CA INDEX NAME)

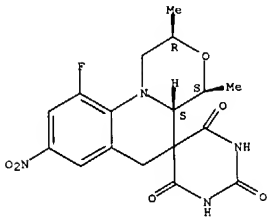
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-66-5 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 10-fluoro-1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

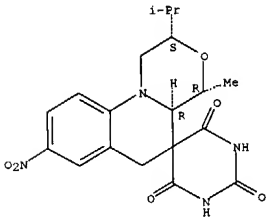
Absolute stereochemistry.



RN 679840-67-6 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-[5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl]-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

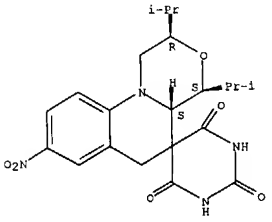
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-70-1 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-bis(1-methylethyl)-8-nitro-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

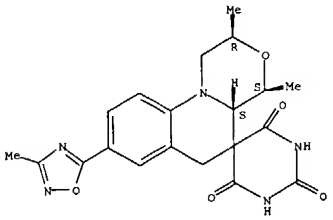
Absolute stereochemistry.



RN 679840-71-2 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(3-methyl-1,2,4-oxadiazol-5-yl)-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

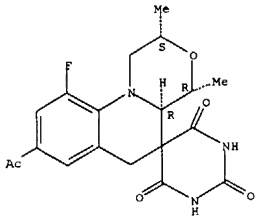
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



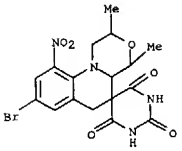
RN 679840-72-3 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-acetyl-10-fluoro-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2S,4R,4aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



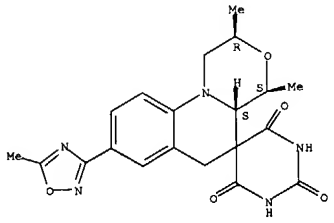
RN 679840-74-5 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-10-nitro- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-75-6 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(5-methyl-1,2,4-oxadiazol-3-yl)-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

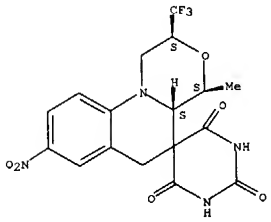
Absolute stereochemistry.



RN 679840-76-7 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-4-methyl-8-nitro-2-(trifluoromethyl)-, (2S,4S,4aS)- (9CI) (CA INDEX NAME)

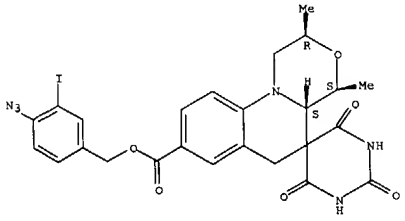
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-77-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8-carboxylic acid, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-, (4-azido-3-iodophenyl)methyl ester, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

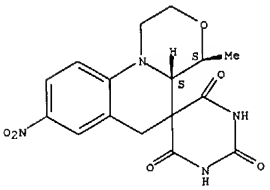
Absolute stereochemistry.



RN 679840-78-9 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-4-methyl-8-nitro-, (4R,4aR)-rel-(-)- (9CI) (CA INDEX NAME)

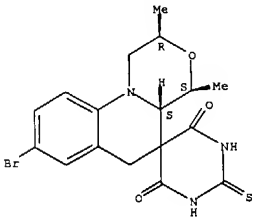
Rotation (-). Absolute stereochemistry unknown.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-79-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-4',6'(1'H,3'H)-dione, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-2'-thioxo-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

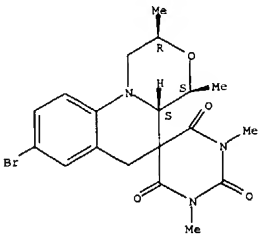
Absolute stereochemistry.



RN 679840-80-3 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-bromo-1,2,4,4a-tetrahydro-1',2,3',4-tetramethyl-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

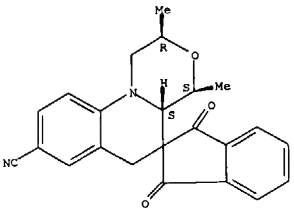
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-81-4 CAPLUS
CN Spiro[2H-indene-2,5'(6'H)-[1,4]oxazino[4,3-a]quinoline]-8'-carbonitrile, 1,1',2',3,4',4'a-hexahydro-2',4'-dimethyl-1,3-dioxo-, (2'R,4'S,4'aS)- (9CI) (CA INDEX NAME)

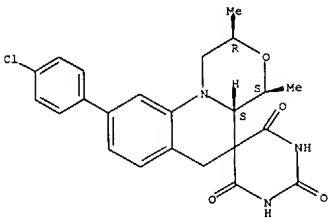
Absolute stereochemistry.



RN 679840-82-5 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5,8(6H)-tricarbonitrile, 1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

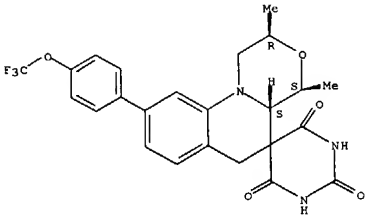
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-86-9 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-[4-(trifluoromethoxy)phenyl]-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

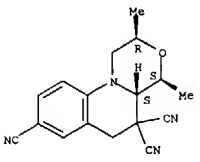
Absolute stereochemistry.



RN 679840-88-1 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-9-(4-methoxyphenyl)-2,4-dimethyl-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

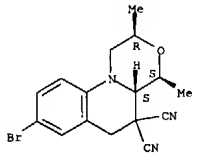
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-83-6 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

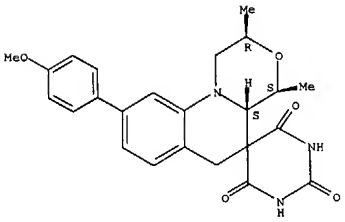
Absolute stereochemistry.



RN 679840-85-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 9-(4-chlorophenyl)-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

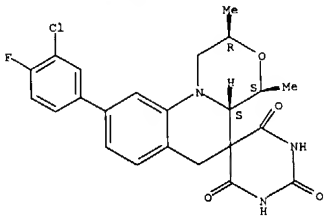
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-89-2 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione,
9-(3-chloro-4-fluorophenyl)-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

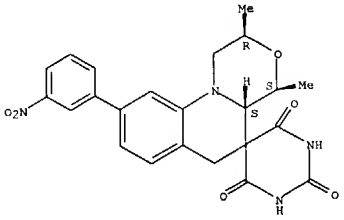
Absolute stereochemistry.



RN 679840-90-5 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-(3-nitrophenyl)-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

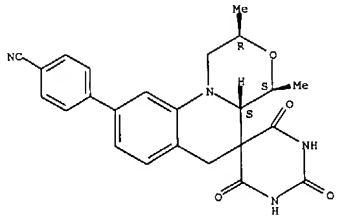
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-91-6 CAPLUS
CN Benzonitrile, 4-[(2R,4S,4aS)-1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-9-yl]- (9CI) (CA INDEX NAME)

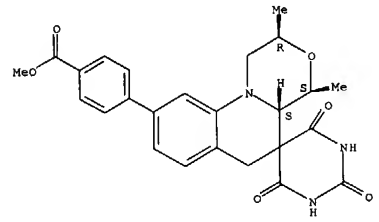
Absolute stereochemistry.



RN 679840-92-7 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-[4-(methylsulfonyl)phenyl]-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

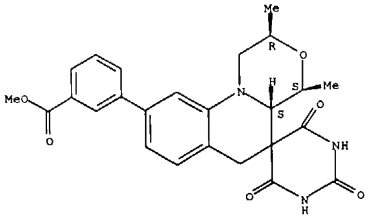
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-95-0 CAPLUS
CN Benzoic acid, 3-[(2R,4S,4aS)-1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-9-yl]-, methyl ester (9CI) (CA INDEX NAME)

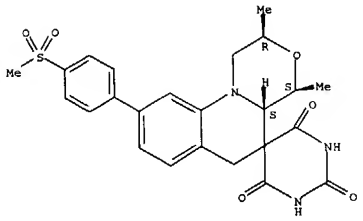
Absolute stereochemistry.



RN 681006-33-7 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

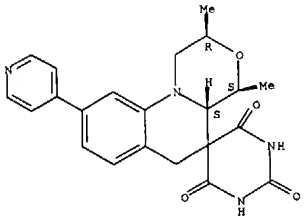
Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679840-93-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-(4-pyridinyl)-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

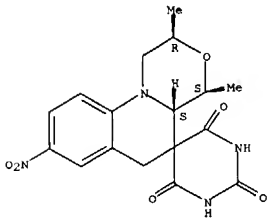
Absolute stereochemistry.



RN 679840-94-9 CAPLUS
CN Benzoic acid, 4-[(2R,4S,4aS)-1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-9-yl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



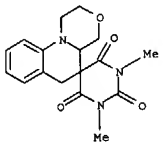
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:43955 CAPLUS
DOCUMENT NUMBER: 140:286965
TITLE: Thermochemical study on the ring closure reaction of 5-morpholino-4-vinylpyridazinones by tert-amino effect
AUTHOR(S): Karolyhazy, Laszlo; Regdon, Geza; Elias, Oliver; Beke, Gyula; Tabi, Tamas; Hodi, Klara; Eros, Istvan; Matyus, Peter
CORPORATE SOURCE: Department of Organic Chemistry, Semmelweis University, Budapest, 1092, Hung.
SOURCE: THEOCHEM (2003), 666-667, 667-680
CODEN: THEODJ; ISSN: 0166-1280
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Cyclization of tert-anilines with a properly substituted vinyl moiety by the tert-amino effect affords fused pyridines. This type of ring closure reaction of 5-morpholino-4-vinylpyridazinones and a benzene analog was investigated by differential scanning calorimetry (DSC) measurements. The structure of products was confirmed by spectroscopic and microanal. methods. The enthalpy values and heats of reactions were obtained from the thermograms by integrating the peak area corresponding to the ring-closure reaction, and by semiempirical (PM3) and DFT (d. function theory) calcns., resp.

IT **675597-19-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (melting temperature; DSC and PM3 and DFT study on the thermochem. of ring closure reaction of 5-morpholino-4-vinylpyridazinones induced by tert-amino effect)

RN 675597-19-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-1',3'-dimethyl- (9CI) (CA INDEX NAME)



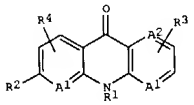
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L4 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:468342 CAPLUS
DOCUMENT NUMBER: 131:102292
TITLE: Preparation of 6-heterocyclyl-9,10-dihydro-9-acridinone derivatives and their nitrogen-containing tri- and tetracyclic analogs as antiviral agents
INVENTOR(S): Furuta, Yosuke; Sugita, Atsushi; Uehara, Sayuri; Takahashi, Kazumi; Nagaki, Hideyoshi; Kamina, Hiroshi; Shiraki, Kimiyasu
PATENT ASSIGNEE(S): Toyama Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 74 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11199565	A2	19990727	JP 1998-294339	19981016
PRIORITY APPLN. INFO.:			JP 1997-303545	19971017

OTHER SOURCE(S): MARPAT 131:102292
GI



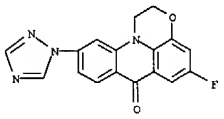
I

AB The title compds. [I; R1 = (un)substituted alkyl, alkenyl, cycloalkyl, aryl, or heterocyclyl; R2 = (un)substituted aryl or heterocyclyl; R3 = H, halo, (un)protected OH, NH2, or CO2H, (un)substituted alkyl; R4 = H, halo; A1, A2 = N, CH; A3 = CH or A3 and R1 together form optionally alkyl-substituted CH2CH2-B; B = O, NH] are prepared They are useful as antiviral agents, in particular anti-herpes simplex virus (anti-HSV) agents. Thus, (10-bromo-5-fluoro-7-oxo-1,2-dihydro-7H-[1,4]oxazino[2,3,4-de]acridin-2-yl)methyl acetate was coupled with 2-(1,1,1-trimethylstannyl)-1,3-thiazole in the presence of bis(triphenylphosphine)palladium dichloride in xylene under reflux, followed by saponification to give 5-fluoro-2-(hydroxymethyl)-10-(1,3-thiazol-2-yl)-1,2-dihydro-7H-[1,4]oxazino[2,3,4-de]acridin-7-one (II). II in vitro inhibited HSV-2 with IC50 of 0.08 μg/mL. Pharmaceutical formulations containing I were also prepared

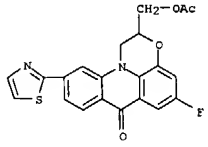
IT **231625-08-4P 231625-10-8P 231625-11-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclyldihydroacridinone derivs. and their

L4 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
nitrogen-contg. tri- and tetracyclic analogs as antiviral agents)

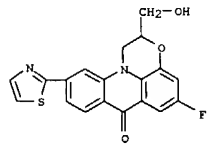
RN 231625-08-4 CAPLUS
CN 7H-[1,4]Oxazino[2,3,4-de]acridin-7-one, 5-fluoro-1,2-dihydro-10-(1H-1,2,4-triazol-1-yl)- (9CI) (CA INDEX NAME)



RN 231625-10-8 CAPLUS
CN 7H-[1,4]Oxazino[2,3,4-de]acridin-7-one, 2-[(acetyloxy)methyl]-5-fluoro-1,2-dihydro-10-(2-thiazolyl)- (9CI) (CA INDEX NAME)



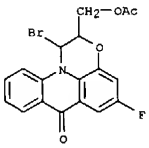
RN 231625-11-9 CAPLUS
CN 7H-[1,4]Oxazino[2,3,4-de]acridin-7-one, 5-fluoro-1,2-dihydro-2-(hydroxymethyl)-10-(2-thiazolyl)- (9CI) (CA INDEX NAME)



IT **231626-13-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heterocyclyldihydroacridinone derivs. and their nitrogen-containing tri- and tetracyclic analogs as antiviral agents)

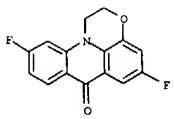
RN 231626-13-4 CAPLUS
CN 7H-[1,4]Oxazino[2,3,4-de]acridin-7-one, 2-[(acetyloxy)methyl]-1-bromo-5-fluoro-1,2-dihydro- (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

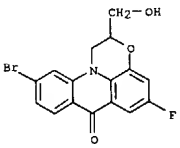


IT **231625-90-4P 231625-98-2P 231625-99-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclyldihydroacridinone derivs. and their nitrogen-containing tri- and tetracyclic analogs as antiviral agents)

RN 231625-90-4 CAPLUS
CN 7H-[1,4]Oxazino[2,3,4-de]acridin-7-one, 5,10-difluoro-1,2-dihydro- (9CI) (CA INDEX NAME)

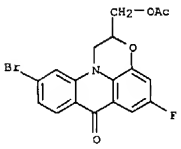


RN 231625-98-2 CAPLUS
CN 7H-[1,4]Oxazino[2,3,4-de]acridin-7-one, 10-bromo-5-fluoro-1,2-dihydro- (9CI) (CA INDEX NAME)



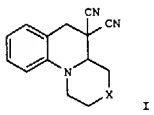
RN 231625-99-3 CAPLUS
CN 7H-[1,4]Oxazino[2,3,4-de]acridin-7-one, 2-[(acetyloxy)methyl]-10-bromo-5-fluoro-1,2-dihydro- (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L4 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:711926 CAPLUS
DOCUMENT NUMBER: 123:285825
TITLE: Synthesis of tricyclic cyano-substituted tetrahydroquinolines by radical decyanation of geminal dinitriles
AUTHOR(S): Gerlach, Uwe
CORPORATE SOURCE: Hoechst AG, Frankfurt, 65296, Germany
SOURCE: Tetrahedron Letters (1995), 36(29), 5159-62
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:285825
GI

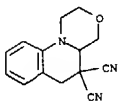


I

AB Various dicyanides I (X = bond, CH2, NMe, O, S, SO, SO2) of tricyclic tetrahydroquinoline derivs. were converted to their monocyanides in high yield by reductive radical decyanation with tributyltin hydride and 2,2'-azobisisobutyronitrile (AIBN).

IT **87699-07-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of tricyclic cyano-substituted tetrahydroquinolines by radical decyanation of geminal dinitriles)

RN 87699-07-8 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 1,2,4,4a-tetrahydro- (9CI) (CA INDEX NAME)

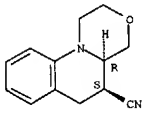


IT **169778-23-8P 169778-24-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of tricyclic cyano-substituted tetrahydroquinolines by radical decyanation of geminal dinitriles)

RN 169778-23-8 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5-carbonitrile, 1,2,4,4a,5,6-hexahydro-, trans- (9CI) (CA INDEX NAME)

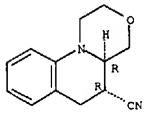
Relative stereochemistry.

L4 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

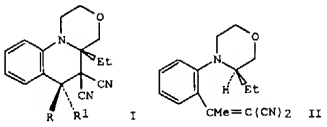


RN 169778-24-9 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5-carbonitrile, 1,2,4,4a,5,6-hexahydro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



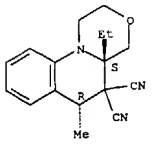
L4 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:38857 CAPLUS
DOCUMENT NUMBER: 110:38857
TITLE: Stereochemical aspects of the "tert-amino effect". 2. Enantio- and diastereoselectivity in the synthesis of quinolines, pyrrolo[1,2-a]quinolines, and [1,4]oxazino[4,3-a]quinolines
AUTHOR(S): Nijhuis, Walter H. N.; Verboom, Willem; Abu El-Fadl, A.; Van Hummel, Gerrit J.; Reinhoudt, David N.
CORPORATE SOURCE: Lab. Org. Chem., Univ. Twente, Enschede, 7500 AE, Neth.
SOURCE: Journal of Organic Chemistry (1989), 54(1), 209-16
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:38857
GI



AB Thermal isomerization of the optically pure 2-vinyl-N,N-dialkylanilines, with a Me or an E substituent at the α-position of the N,N-dialkyl moiety, affords enantioselectively the optically pure pyrrolo[1,2-a]quinolines and the [1,4]oxazino[4,3-a]quinoline, with the Me or Et substituent at the bridgehead C atom, and the quinoline, resp. The optical purity of these quinoline derivs. was determined by 1H-NMR spectroscopy in the presence of chiral shift reagents. Heating of the optically pure analogs in which the substituent is a methoxymethyl group in refluxing 1-butanol yields, besides the compds. with the methoxymethyl group at the bridgehead carbon atom, also the regioisomers that are enantiomerically pure. Mixts. of the diastereomers e.g. I (R, R1 = H, Me) were obtained by cyclization of compound e.g. II, with a 3-ethylmorpholinyl group, in refluxing 1-butanol. The compds. were proven enantiomerically pure. The configuration of the compds. were determined by x-ray anal. of I (R = H, R1 = Me) and 1H-NMR, and 1H-NOE difference spectroscopy. These results provide conclusive evidence for the mechanism of these cyclization reactions, which are further examples of the "tert-amino effect". The effect of substituents on the enantio- and diastereoselectivity of the cyclization is discussed.
IT **117607-21-3P 117607-28-0P**

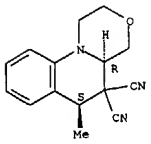
L4 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and crystal structure of)
RN 117607-21-3 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 117607-28-0 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 1,2,4,4a-tetrahydro-6-methyl-, trans- (9CI) (CA INDEX NAME)

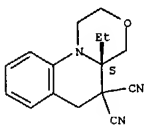
Relative stereochemistry.



IT **117607-20-2P 117607-22-4P 117677-89-1P 117677-90-4P**
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
RN 117607-20-2 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-, (S)- (9CI) (CA INDEX NAME)

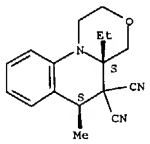
Absolute stereochemistry.

L4 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



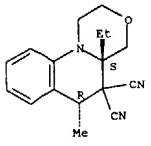
RN 117607-22-4 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 117677-89-1 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, (4aS-trans)- (9CI) (CA INDEX NAME)

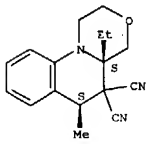
Absolute stereochemistry.



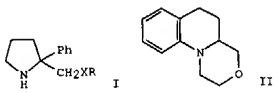
RN 117677-90-4 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

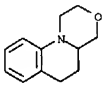


L4 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:611257 CAPLUS
DOCUMENT NUMBER: 101:211257
TITLE: A novel method for heteroatom-substituted free radical generation by photochemical electron transfer induced desilylation of RXCH2SiMe3 systems
AUTHOR(S): Brumfield, Martha A.; Quillen, Suzanne L.; Yoon, Ung Chan; Mariano, Patrick S.
CORPORATE SOURCE: Dep. Chem., Univ. Maryland, College Park, MD, 20742, USA
SOURCE: Journal of the American Chemical Society (1984), 106(22), 6855-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



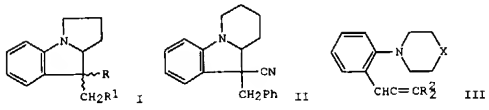
AB Irradiation of 2-phenyl-1-pyrrolinium perchlorate in MeCN containing RXCH2SiMe3 (RX = EtO, Me2CHO, EtS) leads to generation of the corresponding adducts I (same RX), arising by pathways involving excitation, singlet state electron transfer, cation radical desilylation, and ultimate radical pair coupling. Similarly, intramol. processes proceeding through these routes lead to production of heterocyclic products. Thus, (trimethylsilylmethoxyalkyl)quinolinium salts produce cyclic ethers, e.g., II, when irradiated in MeCN, followed by hydrogenation.

IT **40971-38-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40971-38-8 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

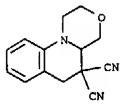
L4 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:51477 CAPLUS
DOCUMENT NUMBER: 100:51477
TITLE: "Tert-Amino effect" in heterocyclic synthesis. Formation of N heterocycles by ring-closure reactions of substituted 2-vinyl-N,N-dialkylanilines
AUTHOR(S): Verboom, Willem; Reinhoudt, David N.; Visser, Richard; Harkema, Sybolt
CORPORATE SOURCE: Twente Univ. Technol., Enschede, 7500 AE, Neth.
SOURCE: Journal of Organic Chemistry (1984), 49(2), 269-76
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:51477
GI



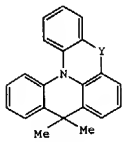
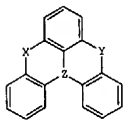
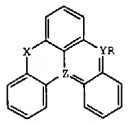
AB 2-Vinyl-N,N-dialkylanilines react thermally in polar solvents and/or in the presence of Lewis acids via [1,5] or [1,6] hydrogen transfer followed by C-C bond formation to give heterotricyclic compds. The reaction depends on the type of N,N-dialkylamino group and on the type and position of substituents of the vinyl moiety. Di-Me 1-pyrrolidinyl butenedioate and (1-pyrrolidinyl)benzeneacetonitrile undergo a thermal rearrangement to the pyrrolo[1,2-a]indoles I (R = R1 = CO2Me; R = cyano, R1 = Ph), resp., while the 1-piperidinyl and 4-morpholinyl butenedioates and (4-morpholinyl)benzeneacetonitrile do not react. (1-Piperidinyl)benzeneacetonitrile yields in refluxing PhMe in the presence of ZnCl2 the pyrido[1,2-a]indole II and its HCN elimination product. Under these conditions cis- and trans-I (R = cyano, R1 = Ph) also eliminate HCN. Heating the III (R2 = CO2Me, cyano, X = bond; R2 = cyano, X = CH2, O) in BuOH gives pyrrolo[1,2-a]quinolines, benzo[c]quinolizine, and [1,4]oxazino[4,3-a]quinoline derivs., resp. The mechanisms of both types of cyclization, which are examples of the tert-amino effect, are discussed.

IT **87699-07-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 87699-07-8 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 1,2,4,4a-tetrahydro- (9CI) (CA INDEX NAME)

L4 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

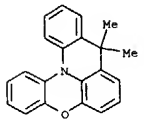


L4 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1980:146175 CAPLUS
DOCUMENT NUMBER: 92:146175
TITLE: Modified tetrahelicene systems. III. Doubly ortho-bridged triphenylamine derivatives
AUTHOR(S): Hellwinkel, Dieter; Schmidt, Werner
CORPORATE SOURCE: Org. Chem. Inst., Univ. Heidelberg, Heidelberg, D-6900/1, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1980), 113(1), 358-84
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 92:146175
GI

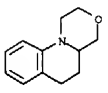

I

II

III

AB Heterocyclic derivs. (e.g., I; Y = PhCMe, CO, CS, CH2, NEt, O, S) or naphth[3,2,1-dc]anthracenes, which can be represented by skeleton types II (X = methylene group, CO; Y = S, methylene or imino group, CS, CO, O, bond; Z = N, C+, C-) or III (X = methylene group, Y = C, Z = N+, C; R undefined), are helically distorted in the stereochem. ground state. They racemize so fast, however, that their free enthalpy of racemization (ΔG ≤21 kcal/mol) can be determined by standard dynamic NMR methods. Only type I compds. with relatively large bridges (Y = PhCMe or S) exhibit higher racemization barriers. The latter had to be determined by classical equilibrium methods. The results indicate that for II and III enlargement of bridges Y and/or X and diminution of Z should increase nonbonding interactions in the planar transition state and therefore increase the racemization barrier. For substituted I (Y = CMe2) derivs., 1H NMR signals of diastereotropic and constitutopic groups were found to coincide.
IT **73183-70-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 73183-70-7 CAPLUS
CN 9H-Quino[3,2,1-kl]phenoxazine, 9,9-dimethyl- (9CI) (CA INDEX NAME)

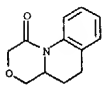
L4 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L4 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1973:124521 CAPLUS
DOCUMENT NUMBER: 78:124521
TITLE: Synthesis of 1,2,4,4a,5,6-hexahydro-1,4-oxazino[3,4-a]quinolines
AUTHOR(S): Rao, V. Aruna; Jain, Padam C.; Anand, Nitya
CORPORATE SOURCE: Cent. Drug Res. Inst., Lucknow, India
SOURCE: Indian Journal of Chemistry (1972), 10(12), 1134-5
CODEN: IJOCAP; ISSN: 0019-5103
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 1,2,4,4a,5,6-Hexahydro-1,4-oxazino[3,4-a]quinoline (I R = H) and its 2-methyl- and 2-phenyl derivs. have been synthesized starting from Me 1,2,3,4-tetrahydroquinaldate (II). II on LiAlH4 reduction, followed by treatment with ethylene oxide, gives 1-β-hydroxyethyl-2-hydroxymethyl-1,2,3,4-tetrahydroquinoline (III, R = H). The latter on treatment with 48% HBr gives I (R = H). Condensation of 2-hydroxymethyl-1,2,3,4-tetrahydroquinoline with styrene and propylene oxides gives the corresponding III (R = Ph, Me), which react with 48% HBr to give the corresponding I as mixts. of diastereoisomers. The stereochem. of the substituents at 2-position has been proposed on the basis of NMR data.
IT **40971-38-8P 40971-39-9P 40971-42-4P**
40971-43-5P 40971-44-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40971-38-8 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro- (9CI) (CA INDEX NAME)



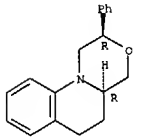
RN 40971-39-9 CAPLUS
CN [1,4]Oxazino[4,3-a]quinolin-1(2H)-one, 4,4a,5,6-tetrahydro- (9CI) (CA INDEX NAME)



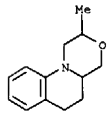
RN 40971-42-4 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro-2-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

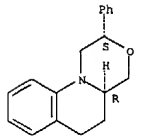


RN 40971-43-5 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro-2-methyl- (9CI) (CA INDEX NAME)



RN 40971-44-6 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro-2-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

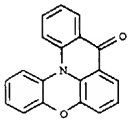


L4 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1968:69015 CAPLUS
DOCUMENT NUMBER: 68:69015
TITLE: Pentacyclic fused ring amines
INVENTOR(S): Zirkle, Charles L.
PATENT ASSIGNEE(S): Smith Kline and French Laboratories
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3337545		19670822	US	19650624

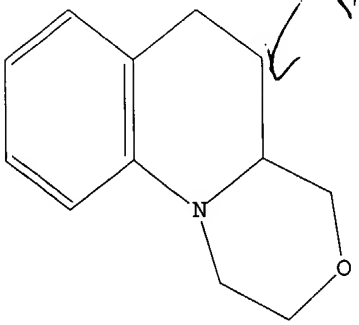
GI For diagram(s), see printed CA Issue.
AB A mixture containing 6.6 g. Me2N(CH2)3Cl, 1.3 g. Mg, and 150-200 ml. anhydrous tetrahydrofuran is refluxed 1 hr. To the mixture is slowly added 9.8 g. 8H-indolo[3,2,2-de]acridan-8-one and the mixture refluxed 4-5 hrs. to give I [R = Me2N(CH2)3 (A), X = OH, Y = H]; I.HCl (II), m. 127°. A mixture containing 6 g. I, 60 g. HCO2Na, and 180 ml. 98% HCO2H is refluxed 24 hrs. to give I [R = A, X = H, Y = H] (III), b0.25 215-18°. II is similarly treated with HCO4H and HCO2Na to give III. I is twice distilled at 0.01-0.1 mm. to give I [(RX =) Me2NCH2CH2CH, Y = H] (IV). Hydrogenation of IV over Pd-on-charcoal in EtOH gives III. Similarly prepared is V (R = A, X = OH, Y = H) m. 182° (decomposition). A stirred mixture containing 13.2 g. o-IC6H4CO2Me 9.2 g. phenoxazine, 6 ml. nitrobenzene, 7.5 g. K2CO3, 85 ml. xylene, and 0.2 g. Cu bronze is refluxed 14 hrs. to give 10-(o-carbomethoxyphenyl)phenoxazine (VI). A suspension containing 6.3 g. VI and 125 ml. 15% aqueous KOH is refluxed 5 hrs. and acidified to give 10-(o-carboxyphenyl)phenoxazine (VII). To a suspension of 1.5 g. VII in 60 ml. xylene is added 1.4 g. PCl5 and the mixture stirred at room temperature for 10 min. The solution is cooled, and a solution containing 6.25 g. SnCl4 and 20 ml. xylene is added dropwise in 10 min. The mixture is stirred 45 min. and hydrolyzed by dropwise addition of 25 ml. cold concentrated HCl to give 9H-quino[3,2,1-kl]phenoxazin-9-one (VIII). VIII is treated as described above to give IX (R, X given): 3-(4-methylpiperazino)propyl (B), OH; and B, H. The compds. are useful as antidepressants.
IT **17591-85-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 17591-85-4 CAPLUS
CN 9H-Quino[3,2,1-kl]phenoxazin-9-one (8CI) (CA INDEX NAME)

L4 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



1

```
=> d l1
L1 HAS NO ANSWERS
L1                STR
```



ring isolated

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 11:46:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    409 TO ITERATE

100.0% PROCESSED     409 ITERATIONS                          2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:         6967 TO     9393
PROJECTED ANSWERS:               2 TO      124

L2             2 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 11:47:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   7865 TO ITERATE

100.0% PROCESSED    7865 ITERATIONS                         20 ANSWERS
SEARCH TIME: 00.00.01

L3            20 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                              ENTRY     SESSION
FULL ESTIMATED COST                           155.42     155.63

FILE 'CAPLUS' ENTERED AT 11:47:09 ON 27 OCT 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
```

FILE COVERS 1907 - 27 Oct 2004 VOL 141 ISS 18
FILE LAST UPDATED: 26 Oct 2004 (20041026/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 6 L3

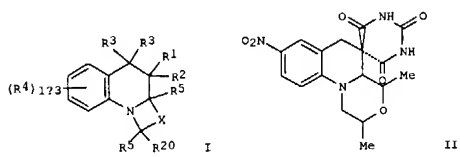
=> d ibib abs hitstr tot

own work

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:308443 CAPLUS
DOCUMENT NUMBER: 140:339202
TITLE: Preparation of tricyclic tetrahydroquinoline antibacterial agents
INVENTOR(S): Barbachyn, Michel Robert; Dobrowolski, Paul Joseph; Hurd, Alexander Ross; McNamara, Dennis Joseph; Palmer, John Raymond; Romero, Arthur Glenn; Ruble, James Craig; Sherry, Debra Ann; Thomasco, Lisa Marie; Toogood, Peter Laurence
PATENT ASSIGNEE(S): Pharmacia & Upjohn Company, USA
SOURCE: PCT Int. Appl., 128 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004031195	A1	20040415	WO 2003-IB4389		20031003
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
US 2004162279	A1	20040819	US 2003-677551		20031002
PRIORITY APPLN. INFO.:			US 2002-416685P	P	20021007
			US 2002-427189P	P	20021118
			US 2003-457622P	P	20030326

OTHER SOURCE(S): MARPAT 140:339202
GI



L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

AB The invention includes tricyclic tetrahydroquinolines (shown as I; variables defined below; many of the examples are spiro compds., e.g. cis- and trans-II), and pharmaceutical compns. thereof, that exhibit useful antibacterial activity against a wide range of human and veterinary pathogens. For I: R1 is R12, C(O)R6, or CN; R2 = R12, C(O)R7, CN, CH2R7, NR17R7, CH2COR7, CH2CH2COR7; R3 = H, R2, O, C1-7 alkyl, C3-8 cycloalkyl, aryl, heteroaryl, or halo; each R4 = H, halo, OR12, OC(O)NR9R10, SR12, S(O)mR13, NR9R10, NR9S(O)mR13, NR9C(O)OR13, Ph, heteroaryl, cyano, nitro, CONR9R10, CO2R12, C(O)R13, C(:NOR12)R13, S(O)mNR9R10, NR9C(O)R12, C1-7 alkyl, C3-8 cycloalkyl, N3, het1, or C(O)O-C1-4alkyl-R12; each R5 = H, C1-7alkyl, C3-8cycloalkyl, aryl or heteroaryl;. X = -[C(R15)2]n-, -[C(R15)2]m-O-[C(R15)2]k-, -[C(R15)2]m-S(O)m-[C(R15)2]k-, or -[C(R15)2]m-NR16-[C(R15)2]k-; R20 is H, C1-7alkyl, C3-8cycloalkyl, aryl, or heteroaryl; Het1 is a C- or N-linked 5-8 membered mono- or bicyclic ring, each mono- or bicyclic ring being fully saturated or partially unsatd., and having 1-4 heteroatoms O, S, and N; het1 being (un)substituted by 1-2 substituents = C1-C4alkyl, amino, C1-C4alkylamino, C1-C4alkyloxy, halogen, CN, O, or S; addnl. details including provisos are given in the claims. A method of preparation is claimed and .apprx.60 example prepns. are included. For example, cis- and trans-II were prepared in 3 steps starting with condensation of 2-fluoro-5-nitrobenzaldehyde with 2,6-dimethylmorpholine to give cis- and trans-2-(2,6-dimethylmorpholin-4-yl)-5-nitrobenzaldehyde, each of which was condensed with barbituric acid to give cis- and trans-5-[2-(2,6-dimethylmorpholin-4-yl)-5-nitrobenzylidene]pyrimidine-2,4,6(1H,3H,5H)-trione, resp., each of which was cyclized in refluxing MeOH. Inhibition of E. coli DNA gyrase by 12 examples of I are reported.

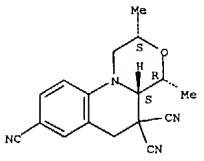
IT **679839-64-6P 679839-65-7P 679840-51-8P 679840-52-9P 679840-82-5P 679840-83-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of tricyclic tetrahydroquinoline antibacterial agents)

RN 679839-64-6 CAPLUS

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

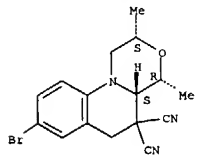
CN [1,4]Oxazino[4,3-a]quinoline-5,5,8(6H)-tricarbonitrile, 1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

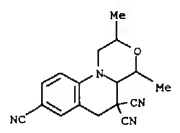


RN 679839-65-7 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

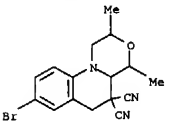


RN 679840-51-8 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5,8(6H)-tricarbonitrile, 1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)



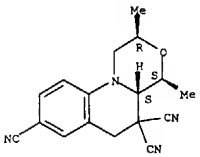
RN 679840-52-9 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



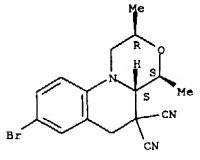
RN 679840-82-5 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5,8(6H)-tricarbonitrile, 1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 679840-83-6 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

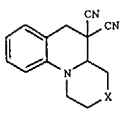
Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:711926 CAPLUS
DOCUMENT NUMBER: 123:285825
TITLE: Synthesis of tricyclic cyano-substituted tetrahydroquinolines by radical decyanation of geminal dinitriles
AUTHOR(S): Gerlach, Uwe
CORPORATE SOURCE: Hoechst AG, Frankfurt, 65296, Germany
SOURCE: Tetrahedron Letters (1995), 36(29), 5159-62
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:285825
GI

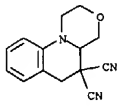


I

AB Various dicyanides I (X = bond, CH2, NMe, O, S, SO, SO2) of tricyclic tetrahydroquinoline derivs. were converted to their monocyanides in high yield by reductive radical decyanation with tributyltin hydride and 2,2'-azobisisobutyronitrile (AIBN).

IT **87699-07-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of tricyclic cyano-substituted tetrahydroquinolines by radical decyanation of geminal dinitriles)

RN 87699-07-8 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 1,2,4,4a-tetrahydro- (9CI) (CA INDEX NAME)

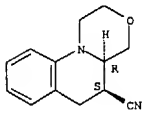


IT **169778-23-8P 169778-24-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of tricyclic cyano-substituted tetrahydroquinolines by radical decyanation of geminal dinitriles)

RN 169778-23-8 CAPLUS

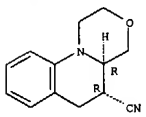
L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN [1,4]Oxazino[4,3-a]quinoline-5-carbonitrile, 1,2,4,4a,5,6-hexahydro-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

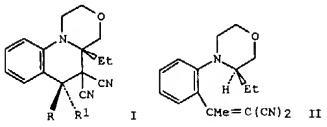


RN 169778-24-9 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5-carbonitrile, 1,2,4,4a,5,6-hexahydro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:38857 CAPLUS
DOCUMENT NUMBER: 110:38857
TITLE: Stereochemical aspects of the "tert-amino effect". 2. Enantio- and diastereoselectivity in the synthesis of quinolines, pyrrolo[1,2-a]quinolines, and [1,4]oxazino[4,3-a]quinolines
AUTHOR(S): Nijhuis, Walter H. N.; Verboom, Willem; Abu El-Fadl, A.; Van Hummel, Gerrit J.; Reinhoudt, David N.
CORPORATE SOURCE: Lab. Org. Chem., Univ. Twente, Enschede, 7500 AE, Neth.
SOURCE: Journal of Organic Chemistry (1989), 54(1), 209-16
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:38857
GI



I II

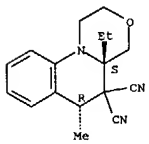
AB Thermal isomerization of the optically pure 2-vinyl-N,N-dialkylanilines, with a Me or an E substituent at the α-position of the N,N-dialkyl moiety, affords enantioselectively the optically pure pyrrolo[1,2-a]quinolines and the [1,4]oxazino[4,3-a]quinoline, with the Me or Et substituent at the bridgehead C atom, and the quinoline, resp. The optical purity of these quinoline derivs. was determined by 1H-NMR spectroscopy in the presence of chiral shift reagents. Heating of the optically pure analogs in which the substituent is a methoxymethyl group in refluxing 1-butanol yields, besides the compds. with the methoxymethyl group at the bridgehead carbon atom, also the regioisomers that are enantiomerically pure. Mixts. of the diastereomers e.g. I (R, R1 = H, Me) were obtained by cyclization of compound e.g. II, with a 3-ethylmorpholinyl group, in refluxing 1-butanol. The compds. were proven enantiomerically pure. The configuration of the compds. were determined by X-ray anal. of I (R = H, R1 = Me) and 1H-NMR, and 1H-NOE difference spectroscopy. These results provide conclusive evidence for the mechanism of these cyclization reactions, which are further examples of the "tert-amino effect". The effect of substituents on the enantio- and diastereoselectivity of the cyclization is discussed.

IT **117607-21-3P 117607-28-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

RN 117607-21-3 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, trans- (9CI) (CA INDEX NAME)

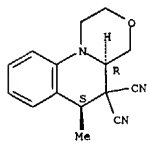
L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Relative stereochemistry.



RN 117607-28-0 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 1,2,4,4a-tetrahydro-6-methyl-, trans- (9CI) (CA INDEX NAME)

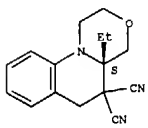
Relative stereochemistry.



IT **117607-20-2P 117607-22-4P 117677-89-1P 117677-90-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 117607-20-2 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-, (S)- (9CI) (CA INDEX NAME)

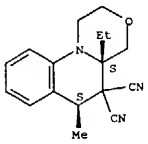
Absolute stereochemistry.



RN 117607-22-4 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, cis- (9CI) (CA INDEX NAME)

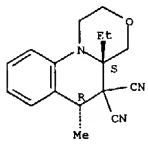
L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Relative stereochemistry.



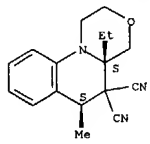
RN 117677-89-1 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, (4aS-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



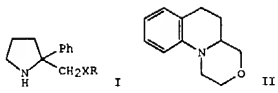
RN 117677-90-4 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

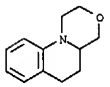


L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

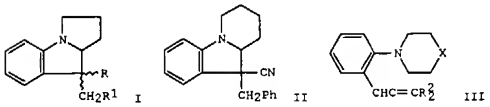
L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:611257 CAPLUS
DOCUMENT NUMBER: 101:211257
TITLE: A novel method for heteroatom-substituted free radical generation by photochemical electron transfer induced desilylation of RXCH2SiMe3 systems
AUTHOR(S): Brumfield, Martha A.; Quillen, Suzanne L.; Yoon, Ung Chan; Mariano, Patrick S.
CORPORATE SOURCE: Dep. Chem., Univ. Maryland, College Park, MD, 20742, USA
SOURCE: Journal of the American Chemical Society (1984), 106(22), 6855-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Irradiation of 2-phenyl-1-pyrrolinium perchlorate in MeCN containing RXCH2SiMe3 (RX = EtO, Me2CHO, EtS) leads to generation of the corresponding adducts I (same RX), arising by pathways involving excitation, singlet state electron transfer, cation radical desilylation, and ultimate radical pair coupling. Similarly, intramol. processes proceeding through these routes lead to production of heterocyclic products. Thus, (trimethylsilylmethoxyalkyl)quinolinium salts produce cyclic ethers, e.g., II, when irradiated in MeCN, followed by hydrogenation.
IT **40971-38-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40971-38-8 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro- (9CI) (CA INDEX NAME)

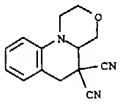


L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:51477 CAPLUS
DOCUMENT NUMBER: 100:51477
TITLE: "Tert-Amino effect" in heterocyclic synthesis. Formation of N heterocycles by ring-closure reactions of substituted 2-vinyl-N,N-dialkylanilines
AUTHOR(S): Verboom, Willem; Reinhoudt, David N.; Visser, Richard; Harkema, Sybolt
CORPORATE SOURCE: Twente Univ. Technol., Enschede, 7500 AE, Neth.
SOURCE: Journal of Organic Chemistry (1984), 49(2), 269-76
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:51477
GI

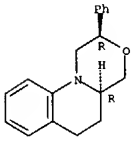


AB 2-Vinyl-N,N-dialkylanilines react thermally in polar solvents and/or in the presence of Lewis acids via [1,5] or [1,6] hydrogen transfer followed by C-C bond formation to give heterotricyclic compds. The reaction depends on the type of N,N-dialkylamino group and on the type and position of substituents of the vinyl moiety. Di-Me 1-pyrrolidinyl butenedioate and (1-pyrrolidinyl)benzeneacetonitrile undergo a thermal rearrangement to the pyrrolo[1,2-a]indoles I (R = R1 = CO2Me; R = cyano, R1 = Ph), resp., while the 1-piperidinyl and 4-morpholinyl butenedioates and (4-morpholinyl)benzeneacetonitrile do not react. (1-Piperidinyl)benzeneacetonitrile yields in refluxing PhMe in the presence of ZnCl2 the pyrido[1,2-a]indole II and its HCN elimination product. Under these conditions cis- and trans-I (R = cyano, R1 = Ph) also eliminate HCN. Heating the III (R2 = CO2Me, cyano, X = bond; R2 = cyano, X = CH2, O) in BuOH gives pyrrolo[1,2-a]quinolines, benzo[c]quinolizine, and [1,4]oxazino[4,3-a]quinoline derivs., resp. The mechanisms of both types of cyclization, which are examples of the tert-amino effect, are discussed.
IT **87699-07-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 87699-07-8 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 1,2,4,4a-tetrahydro- (9CI) (CA INDEX NAME)

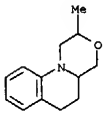
L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Relative stereochemistry.

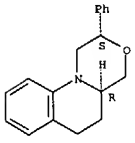


RN 40971-43-5 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro-2-methyl- (9CI) (CA INDEX NAME)

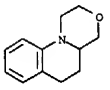


RN 40971-44-6 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro-2-phenyl-, cis- (9CI) (CA INDEX NAME)

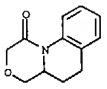
Relative stereochemistry.



L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1973:124521 CAPLUS
DOCUMENT NUMBER: 78:124521
TITLE: Synthesis of 1,2,4,4a,5,6-hexahydro-1,4-oxazino[3,4-a]quinolines
AUTHOR(S): Rao, V. Aruna; Jain, Padam C.; Anand, Nitya
CORPORATE SOURCE: Cent. Drug Res. Inst., Lucknow, India
SOURCE: Indian Journal of Chemistry (1972), 10(12), 1134-5
CODEN: IJOCAP; ISSN: 0019-5103
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 1,2,4,4a,5,6-Hexahydro-1,4-oxazino[3,4-a]quinoline (I R = H) and its 2-methyl- and 2-phenyl derivs. have been synthesized starting from Me 1,2,3,4-tetrahydroquinaldate (II). II on LiAlH4 reduction, followed by treatment with ethylene oxide, gives 1-β-hydroxyethyl-2-hydroxymethyl-1,2,3,4-tetrahydroquinoline (III, R = H). The latter on treatment with 48% HBr gives I (R = H). Condensation of 2-hydroxymethyl-1,2,3,4-tetrahydroquinoline with styrene and propylene oxides gives the corresponding III (R = Ph, Me), which react with 48% HBr to give the corresponding I as mixts. of diastereoisomers. The stereochem. of the substituents at 2-position has been proposed on the basis of NMR data.
IT **40971-38-8P 40971-39-9P 40971-42-4P 40971-43-5P 40971-44-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40971-38-8 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro- (9CI) (CA INDEX NAME)



RN 40971-39-9 CAPLUS
CN [1,4]Oxazino[4,3-a]quinolin-1(2H)-one, 4,4a,5,6-tetrahydro- (9CI) (CA INDEX NAME)



RN 40971-42-4 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro-2-phenyl-, trans- (9CI) (CA INDEX NAME)